ISCR Institute for Scientific Computing Research

Subcontracts, ASCI Level 3

CASC Center for Applied Scientific Computing

Unconditionally Stable Lattice Boltzmann Algorithms for Hydrodynamic Simulation

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Abstract

The term “lattice Boltzmann algorithms” for computational fluid dynamics describes the time evolution of a discrete-velocity distribution function at each lattice point. Moments of these distributions then yield the desired hydrodynamic variables. Conservation of mass, momentum and energy (if appropriate) impose various equality constraints on these distributions, and positively impose various inequality constraints. We propose to use methods of linear algebra to coordinatize the subspace of distribution values that obey the conservation laws, and to use the Fourier-Motzkin elimination method to sequentially bind the coordinates within the polytope thus constructed. By then constructing an entropy function that reaches a maximum within this polytope, and goes to –∞ on its boundaries, and by demanding that the collision process increase this entropy, we can construct unconditionally stable lattice Boltzmann algorithms. Limitations on Reynolds number are then due to a minimum value of the attainable viscosity. We propose that the applicability of algorithms constructed in this way for applications in computational fluid dynamics be investigated.

Institute for Scientific Computing Research

Research on Accelerated Strategic Computing Initiative (ASCI) Applications

David Keyes

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Abstract

The objective of this work is to introduce algorithmic ideas and research software implementations (in the form of the PETSc and PME libraries) useful to the parallelization of structured and unstructured grid PDE applications, implicit and explicit. The goal is to assist with the automation and optimization of parallel ports of "clean" legacy applications.

The work will research the following algorithms in the context of Accelerated Strategic Computing Initiative (ASCI) applications

- Domain decomposition.
- Newton-Krylov-Schwarz (NKS) methods for nonlinear equations.
- Nonlinear multilevel methods.

The researcher shall know how to restructure existing data structures and how to extract the specific expertise and investment in a code, while leaving behind solver-related code that is obsolete in the parallel environment.

Center for Applied Scientific Computing

Algebraic Multigrid (AMG) Software

John Ruge

Front Range Scientific Computation, Inc.

Abstract

The purpose of this project is the development and extensive testing of robust Algebraic Multigrid (AMG) software for solving unstructured-mesh problems that are designed to run in both serial and parallel environments. The emphasis will be on testing existing AMG codes on the problems of interest to Lawrence Livermore National Laboratory (LLNL), especially time-dependent 3D elasticitiplasticity problems and 3D heat conduction–diffusion equations. Another major focus is the design of highly parallel AMG strategies. Several technical approaches to improving AMG robustness and parallelism have been identified and studied in the framework of problems of interest to LLNL. Two major technical achievements were the conceptualization of schemes.